Phase 2 Project Summary

Firm: Intelligent Automation Inc.,

Contract Number: NNX10CB63C

Project Title: HPC Benchmark Suite, NMx

Identification and Significance of Innovation: (Limit 200 words or 2,000 characters whichever is less)

The comprehensive numerical HPC benchmark NMx suite benchmarks current and future high performance computing activities. The HPC benchmark suite NMx includes:

- dense and sparse unsymmetrical matrix problems faced in space aviation and problems in thermally driven structural response and radiation exchange
- implicit solution algorithms with production models and benchmarks for indefinite matrices and pathological cases
- configurations scaling for large systems distributed high performance system in shared, distributed and mixed memory condition
- · available solvers in public and developed solvers for various computing architectures

Technical Objectives and Work Plan: (Limit 200 words or 2,000 characters whichever is less)

- Selection of models with analytical solutions and implicit solution algorithms with indefinite and large sparse and dense matrix conditions
- Selection of problems with precision and round-off studies on serial and parallel machines
- Test implementation and demonstration of the problem set on selected cluster architectures and study wall clock performance with respect to the number of processors
- Comparison of solutions on serial and parallel hardware in different architectures
- Analyze and document the strengths, weaknesses, and limitations of the toolkits used together with recommendations

Work plan:

- Task1. Arrange a kickoff meeting with NASA and understand the requirements for future HPC benchmarking
- Task 2: Perform benchmarks of Sparse and Dense Matrices with routines from ScaLAPACK, PETSc, SuperLU_DIST and GPU based CULA, MAGMA CUDA and MinGPU
- Task 3: Incorporate benchmarked Linear Algebra routines into implicit solution algorithms
- Task 4: Package various permutations of HPC Linear Algebra Libraries for Benchmarking on STOKES
- Task 5: Analyze and document the strengths, weaknesses, and limitations of the toolkits used together with recommendations with selected cluster architectures, wall clock performance with respect to the number of processors.
- Task 6: Packaging various permutations of HPC Linear Algebra Libraries for Benchmarking on various architectures
- Task 7: Technology transition and commercialization

Technical Accomplishments: (Limit 200 words or 2,000 characters whichever is less)

 We have benchmarked large dense and sparse problems that are of interest to NASA under various configurations with public available solver libraries and with our developed solvers. We modified our solvers to use NASA JPL's sparse solver library and benchmarked the model problems.

- Model problems that are sparse and dense and have unsymmetric matrix and that are of interest to NASA in space aviation and thermally driven structural response and radiation exchange were developed using NASTRAN/PATRAN.
- We benchmarked with publicly available PETSc with SuperLU_Dist routine for solving linear system of equations for Thermal Equilibrium of the form, K * □u = r for the most general form K as a dense complex unsymmetric matrix.
- We developed our own biconjugate solver with variations that worked for shared GPU and distributed GPU. We benchmarked the developed realistic model problems and the random generated positive definite problems of various densities.
- The benchmark tool is packaged to run the choice of solver, choosing a particular architecture and set of problems in a configuration that is in the STOKES HPC

NASA Application(s): (Limit 100 words or 1,000 characters whichever is less)

The most promising commercial applications are:

- heat transfer problems in structures in avionics, diagnostic of structures in space exploration and exploration of structure formation and problems in geology
- The tools developed will greatly improve the performance and efficiency to adapt the benchmarks to different hardware architectures to various HPC systems at NASA facilities.
- For NASA other applications include testing requirements for computation architectures where simulation modeling environments have solvers that run into hundreds of degrees of freedom. These include testing of high performance applications in diagnostics and health monitoring applications.

Non-NASA Commercial Application(s): (Limit 200 words or 2,000 characters whichever is less)

- thermal and structural problems in industry, automobiles, manufacturing sectors and military
- Other applications include diagnostics and health monitoring applications
- problems in large scale platforms for high performance simulations in CPU and GPU architectures for civilian use and academics

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